International Journal of Industrial Engineering, 2018;2(9):190-196.
ISSN: 2456-8449.
http://ijie.gjpublications.com

Review Article

Impression on Continuous and Batch Reactors and their Suitable Application for Optimal Operation

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Abstract

The present study has been focused for the design of optimal operations of various reactor networks like batch and continuous reactors with their suitable impeller and feed conditions. The kinetic properties like velocities and viscosities of feeds are plays a major important role in the formation of imminent dead zone in reactor designs and in turn it relates with mixing processes of the impeller. Several variable parameters for the design of the continuous and batch reactors have been studied. Further the accessible parameters like impeller speed, type of impeller, number of impellers, clearance between the impellers, average residence time and the properties of the feed stream have been reported in the present review.

Keywords: Choice of reactor; Impeller types; Operation of reactor; Feed condition.

Introduction

A chemical reactor is one of the major equipment in production plant in which process transformations have been carried out to obtain desired product in the specified rate [1]. Since reactors are very important in the chemical industry, thereby choose of an optimal reactor decides the success or failure of the plant. The reactor configuration and its operating conditions have been selected with proper design and operating constraints to achieve maximum profit and zero discharge of pollutants [2]. The conversion that is realised during the reaction in the reactor largely influences the high cost spent on the separators or the downstream process involved [3].

Based on the type of feed interaction it has been classified as Batch reactor, Semi Batch Reactor and Continuous Stirred Tank Reactor. Further it has been observed that the reaction type and its feed property depend on viscosity, feed rate and concentration, etc [4]. The diversity of the chemical reaction deals with process variables and magnitude level during the process condition. This paper is mainly reviewed the importance of the reactor and significance of its feed types, impellers used, agitation rate, oscillation of concentration and the number of stages required and to specify the necessary constraints to be marked to complete the process.

Batch reactors

Batch reactors are reactors in which no matter enters or leaves the reactor within the stipulated reaction time during which the reaction takes place [5]. So, the operation is inherently an unsteady state operation [6]. These reactors are very common in process industries mainly in the production of fine chemicals, speciality chemicals and polymers. They are extensively used in processes which are newly synthesized, difficult to control or sometimes uneconomical in a continuous reactor [7]. Reactions which have large conversion time, more heat of reaction or involve viscous reactants are reacted through batch wise system. Kinetics and thermal modeling of reactions are also made using batch reactors [8]. The ideal batch operation is not possible if the reaction is highly exothermic or any of the reactant is in gaseous state. The common assumption is that at any instant the reactor has uniform concentration and temperature [9]. The main difference between a batch reactor and a continuous stirred

Received: 03.09.2018; Received after Revision: 18.09.2018; Accepted: 18.09.2018; Published: 28.09.2018

tank reactor is that concentration changes periodically in the former while spatially in the latter. The batch reactor specifies its operation in an extensive path way of high malleability and economically feasibility of the reaction. But those specified and uncontrolled newly synthesised process cannot be operable in continues reactor [10]. Further the process in batch reactor supports the following kinetic parameter like basis of the reaction, constant volume batch reactor in gas phase reactions and constant volume in liquid phase reactions. In add up with the above constraints the batch reactor can also be studied in variable volume of ideal gas condition [11]. If an arbitrary species is the limiting reagent with constant volume condition the design structure for batch reactor is studied clearly by mole balance, rate laws and stoichiometry [4].

Design of the batch reactor

Input = output + disappearance + accumulation (1)

Input = output (2)

$$\left(\begin{matrix}\text{Rate of loss of}\\ \text{reactant due to reaction}\end{matrix}\right) = -\left(\begin{matrix}\text{Rate of loss of}\\ \text{accumulation of reactant A}\end{matrix}\right) \quad (3)$$

Disappearance by Reaction = $(-r_A)V$

$$= \left(\frac{\text{moles of A reacting}}{(\text{time})(\text{volume of fluid})}\right)(\text{volume of fluid}) \quad (4)$$

Accumulation of A = $\frac{dN_A}{dt} = \frac{d[N_{A0}(1-X_A)]}{dt} = -N_{A0}\frac{dX_A}{dt}$ (5)

By eq (1) $(-r_A)V = -N_{A0}\frac{dX_A}{dt}$

Rearranging and integrating

$$t = N_{A0}\int_0^{X_A}\frac{dN_A}{(-rA)V}$$

This is the performance or design equation for a batch reactor.

If the density of the fluid remains constant, we can write the design equation in terms of concentration [12].

$$t = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)}$$

$$t = -\int_{C_{A0}}^{C_A}\frac{dC_A}{(-r_A)}$$

For fluids with varying density we define

$$\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}}$$

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)V_0(1+\varepsilon_A X_A)} = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)} \quad (6)$$

Where,

$V_{X_A=1}$ = Volume at complete conversion

$V_{X_A=0}$ = Volume at no conversion

Similarly for a constant volume of batch reactor the following variables are described

$$\partial = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \quad (7)$$

The total mole is described by

$$N_T = N_{T}o + \partial N_{A}oX \quad (8)$$

A Table 1 like the one below can be used to compute changes and remaining quantities of substances in a constant volume batch reactor.

Table 1. Constant Volume of Batch Reactor

Symbol	Initial	Change	End(Moles)	End(Concentration)
A	N_{Ao}	$-N_{Ao}X$		
B	$N_{Bo} = \Theta_B N_{Ao}$	$-\frac{b}{a}N_{Ao}X$	$N_{Ao}\Theta_B - \frac{b}{a}X$	$C_{Ao}\Theta_B - \frac{b}{a}X$
C	$N_{co} = \Theta_c N_{Ao}$	$-\frac{c}{a}N_{Ao}X$	$N_{Ao}\Theta_c + \frac{c}{a}X$	$C_{Ao}\Theta_C + \frac{c}{a}X$
D	$N_{co} = \Theta_c N_{Ao}$	$-\frac{d}{a}N_{Ao}X$	$N_{Ao}\Theta_D + \frac{d}{a}X$	$C_{Ao}\Theta_D + \frac{d}{a}X$
Total	N_{To}		$N_T = N_{To} - N_{Ao}X$	

$$= C_{Ao}(\Theta_i + v_i X) \quad (9)$$

The bases of the reaction the substance A[13-14] is the limiting reagent and the mole fraction of a definition Θ constant volume batch reactor is given by the eq. (9).

$$C_i = C_{Ao}(1-X) = \frac{NAo[\Theta i \mp (\frac{i}{a})X]}{V}$$

In addition for generation of the product and subtraction for the consumption of the reactant is represented by stoichiometric number of species. The corresponding stoichiometry coefficient is expressed in equation 11 in which

positive for product sides and negative for reactant sides.

$$v_i = \pm \frac{i}{a} \quad (10)$$

For any gas phase reaction, constant volume condition tend to exist when n moles of reactant form n moles of product[15]and when there is no change in temperature or pressure in ideal gas law[16]. For liquid phase reaction, the solvent dominate the solution and hence the density of the solute negligibly impacts the system and making essentially a constant volume conditions as shown in Figure 1.

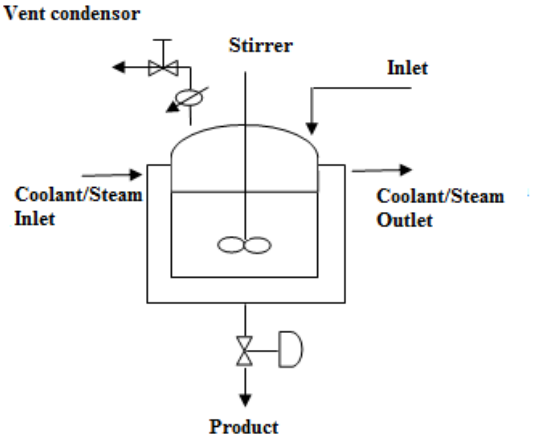

Figure 1. Batch reactor

Continuous reactor

Continuous stirred tank reactor (CSTR)

Continuous stirred tank reactor (CSTR) are the reactors producing constant continuous product by converting continuously fed feed stream as shown in the Figure 2 [17-19]. Continuous stirred tank reactor is a model more than a reactor, comprising of important classes of continuous reactors such as continuous, steady and agitated tank reactors [20]. The model is primarily inherent with two assumptions are steady state operation and uniform operating conditions like retention time of the molecules, concentration and temperature [21]. In general the CSTR are equipped with an agitator in which the mixing is in axial direction. Further if there is increase in the size of the reactor, the mixing decreases [22].

The retention time is the time spent by one reactor volume of continuous feed and its value has been optimised by CFD or simple RTD methods with simple construction [23].

Design of the continuous stirred tank reactor

For a CSTR the design consideration of steady state mass balance equation for the feed is the difference in the feed mass to the mass of the product formed due to the reaction and the rest being the unconverted product recovered at the exit of the reactor [24].

$$F_{i(in)} - r_i V_R = F_{i(out)} \quad (11)$$

For a reaction m involving species i;

$$\sum (S_j)_i r_i V_R = \sum (S_j)_m (X_{m\,out} - X_{m\,in}) \quad (12)$$

The summation in the left is for independent reaction, whereas the summation on the right hand side is for all the reactions taking part in the reaction.

$$F_{i\,in} - F_{i\,out} = \sum (S_j)_m (X_{m\,out} - X_{m\,in}) \quad (13)$$

$$X_{m\,out} - X_{m\,in} = (r_m + \sum k_m r k_{out}) V_R \quad (14)$$

Therefore for a single chemical reaction

$$X_{m\,out} - X_{m\,in} = r V_R \quad (15)$$

$$V_R = F_A (f_{A\,out} - f_{A\,in}) / -r_A \quad (16)$$

$$X_{A\,out} - X_{A\,in} = F_A (f_{A\,out} - f_{A\,in}) \quad (17)$$

Equations 4 and 6 are known as the performance equation of continuous stirred tank reactor.

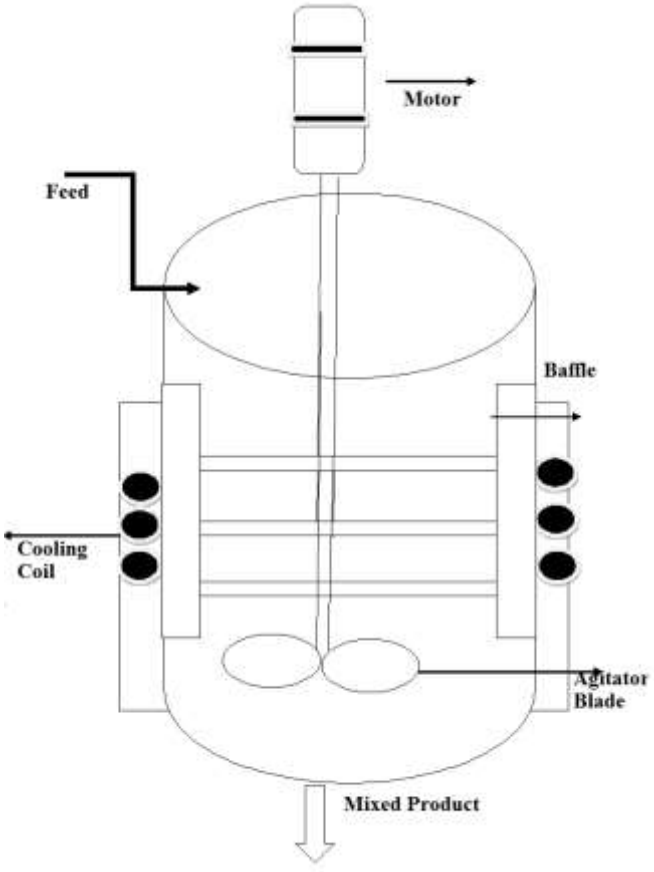

Figure 2. Continuous reactor

Choice of the selection of reactors

The reactors have been selected based on the mode of operation, geometric configuration, contacting patterns and also on the way in which the temperature is to be maintained with

isothermal, non-isothermal or adiabatic operation [25]. In this section the choice of the process are not concerned on the temperature aspect but it depends on property of the fluid, economic aspects and has not depend on the reaction progress [26].

Comparison of reactors

CSTR have more advantages over the other types of the reactors, if the production rates are maintained without any process variables interference like control level of improvement, decreased operating time and periodical cleaning as such in batch reactor [27]. Further the performance of a CSTR is highly dependent on the properties of fluids like hydrodynamics and turbulence levels generated in the vessel. The above significant factors are determined by operating conditions, the agitator, vessel geometry, as well as the positions of the inlet and outlet streams [28]. As compared with batch operation the yield of intermediate product obtained in continuous reactors as a CSTR or cascades are allows the limited tanks of considerably lower concentrations [29]. But sometimes batch operation is difficult, particularly with fast exothermic reactions because of the high rate of reaction and heat release. In such cases CSTRs are used in spite of low production rates. But for very fast exothermic reaction this is not possible such as a gas phase reaction [30]. Although many advantages of the CSTR as par with the batch reactor is reported, but still some inherent constraints like economic optimizations, the size of the production, reaction time, the nature of the process and the yield of the reaction are greatly associated[31]. Further some Semi batch reactor is also used for the fast chemical reaction so that the reaction can be regulated and where the slow chemical reactions are operated and maintained in precise temperature level in the reactor. A combined mode of operation can also be preferred where initially the reaction might be carried in a semi-batch reactor and then extension of reaction under a batch reactor or vice-versa [32].

Economic optimizations

The cost of the equipment has low value in respective with scale of the production as compared to the operating cost of the reactor [33]. The cost analyses have been sorted and it shows that the fixed cost is a linear function [34] with the scale whereas the operating cost is a non-linear function. In growing needs of the demand of the products, a wide opportunities and synergies of the particular products thereby a great increase in operating costs which includes the cost of start up and end up of the process, heat recovery from the effluents, cost of controlling staffs and control equipments[35-36]. Sometimes at high production rates the production may face serious consequences and operating expenses are reaches at higher value than the breakeven point [37].

Size of production

If the size of the equipment increases subsequently the cost of fabrication and transportation has also increases. Further at a rapid rate, the production increases, whereas the cost of control and labour utilization has also increases non-proportionally [38].

Reaction time

The production time of antibiotics takes about 1-2 weeks so in such cases the batch reaction in small scale is preferred. For such cases the CSTR cannot be equipped at all [39]. In the case of a batch reactor with the multi variable optimization model can be used with several process parameters like optimal temperature, coolant flow rate and rate of agitation [40].

Nature of the process

If the reaction process at an exothermic condition there must be generation of heat and simultaneously the heat must be removed from the reactor, in order to maintain the desired reaction temperature [32]. In such cases the cooling water must be sent through the special arrangements inside the reactor and subsequently heating fluid is sent through the heating coils in the reactor for an endothermic reaction [33]. Though this can be recovered with heat recovery systems, the quality of the waste heat form the reactor is not rich, say in fermentation processes the maximum temperature does not increase 70°C within the reactor so the heat recoverable might only be 20°C so installing a separate waste heat recovery system and using the generated heat for the purpose of preheat, might be an additional investment. For the large scale operations it also increases with the pumping level and the labour cost requirements [39].

Rate of mixing

The rate of mixing must always be large as the film diffusion will not be a resisting parameter. Levenspiel's study shows that the N_d value must always be greater than 0.2 [40]. The hydrodynamic distribution expressed in the longitudinal dispersion model will give the optimal range of N_d and provided the dimensionless equation of σ^2. In order to maintain a high mixing rate the N_d value must be larger [38].

$$\sigma^2 = 2{T_d}^2\left[N_d - \left({N_d}^2\left(1 - e^{-1/N_d}\right)\right)\right] \quad (18)$$

Where

$$\sigma^2 = 2\int_0^\infty \left(t\left(1 - \frac{C_t}{C_0}\right)dt\right) - {T_d}^2 \quad (19)$$

Where C_0 is the initial concentration of the substrate

C_t is the concentration after time t

T_d is the hydraulic retention time

Viscosity

Viscosity of the fluids plays an important role in the efficient mixing of the viscous feed. In such cases close clearance impellers can be used to make the whirl [36].Since change in viscosity of the fluid has becomes inefficient for non-Newtonian fluids. For such feeds the impeller is rotated in a particular direction. In non-Newtonian fluids the problem of the viscosity can be countered by two ways like a short circulating time and a mixing zone with a feedback. For non-Newtonian and the pseudo-plastic type fluids the use of an axial impeller causes more channelling and also forms large dead zone volumes and hence Maxblend impeller is to be preferred [39].

Temperature control

In order to maintain the temperature in the reactor the optimized model of preheating and heat recovery system is most essential. This is done with the help of a jacketed vessel. The prime conditions have to be utilised like preheat of the reaction mixture to an extent of temperature, sustain the reaction phase thereby temperature is raised rapidly, and the heat is recovered from the product. For slow heating process, single intermediate medium is to be circulated and the temperature is also maintained using the flow rate of the fluid. For the rapid heating this has to be done with steam-glycol mixture and this mixture which in turns maintains level the temperature inside the reactor [40].

Conclusions

The present review covers the prime importance of certain processes variables and also considered the choice of the selection of the reactor. The choice of process parameters and reactor design for small scale is of less constrained than the selection at the larger scale are also discussed. The problem with some of the reaction for choosing batch reactor must be due to the reaction and the residence time. But with the micro-reactor this constraint can be offset. These micro reactors are said to reduce the reacting time of 5 h operation to mere 10 sec. This complete guidance of the design, selection and the example of operation of batch and continuous reactors might give an overall view of the reactors design and their behaviour itself.

Conflicts of interest

Authors declare no conflict of interest.

References

[1] Friedrich M, Perne R. Design and control of batch reactors: An industrial viewpoint. Comput Chem Eng 1995;19(1):357-68.

[2] Louleh Z, Cabassud M. A new strategy for temperature control of batch reactors: experimental application. Chem Eng J 1999;75(1):11-20.

[3] Donati G, Paludetto R. Batch and semibatch catalytic reactors (from theory to practice). Catal. Today 1999;52(2-3):183-95.

[4] Anyanwu CN, Mbajiorgu CC, Oparaku OU, Odigboh EU, Emmanuel UN. A design algorithm for batch stirred tank transesterification reactors/ Energ Convers Manage 2012;62:40-6.

[5] Aubin J, Kresta SM, Bertrand J, Xuereb C, Fletcher DF. Alternate operating methods for improving the performance of continuous stirred tank reactors. Chem Eng Res Des 2006;84(7):569-82.

[6] Yuan Z, Yang H, Zhi X, Shen J. Increased performance of continuous stirred tank reactor with calcium supplementation, Int. J Hydrogen Energ 2010; 35(7):2622-6.

[7] Aubin J, Mavros P, Fletcher DF, Bertrand J, Xuereb C. Effect of axial agitator configuration (up-pumping, down-pumping, reverse rotation) on flow patterns

generated in stirred vessels, Chem Eng Res Des 2001;79(8):845-56.

[8] Pakzad L, Ein-Mozaffari F, Upreti SR, Lohi A. Evaluation of the mixing of non-Newtonian biopolymer solutions in the reactors equipped with the coaxial mixers through tomography and CFD. Chem Eng J 2013;215-216:279-96.

[9] Aris.R and N.R.Amundson. An analysis of chemical reactor stability and control. Parts I-III. Chem Eng Sci 1958;7:121-55.

[10] Levenspiel O. Chemical Reaction Engineering, Ind Eng Chem Res 1999; 38:4140-43.

[11] Uebel K, Rößger P, Prüfert U, Richter A, Meyer B. A new CO conversion quench reactor design. Fuel Process Technol 2016; 148:198-208.

[12] Lay CH, Huang CY, Chen CC, Lin CY. Biohydrogen production in an anaerobic baffled stacking reactor: Recirculation strategy and substrate concentration effects. Biochem Eng J 2016;109:59-64.

[13] Brooks BW, Kropholler HW, Purt SN. Emulsion polymerization of Styrene in a continuous stirred reactor. Polym J 1978; 19:193-203.

[14] J.Alvarez-Ramrez. Stability of a class of uncertain continous stirred reactors with a non linear feedback. Chem Eng Sci 1994;49(11):1743-48.

[15] Luca C, Massa P, Fenoglio C, Cabello F M. Improved Fe_2O_3/Al_2O_3 as heterogeneous Fenton catalysts for the oxidation of phenol solutions in a continuous reactor. J Chem Technol Biotechnol 2014;89:1121-28.

[16] Patel VR, Ein-Mozaffari F, Upreti SR. Effect of time delays in characterizing the continuous mixing of non-Newtonian fluids in stirred-tank reactors. Chem Eng Res Des 2011;89(10):1919-28.

[17] Baldyga J, Bourne JR, Yang Y. Influence of feed pipe diameter on mesomixing in stirred tank reactors. Chem Eng Sci 1993; 48(19):3383-90.

[18] Filippe C, Greffe J L, Bordet J, Villermaux J, Barne J L, Bonte P, Georgakis G, Tendency modeling of Semibatch reactors for optimization and control. Chem Eng Sci 1986;41:913-20.

[19] Cott BJ, Macchitteo S. Temperature control of exothermic batch reactors using generic model reactor. Ind Eng Chem Res 1989;28:1177-84.

[20] Copelli S, Derudi M, Rota R. Topological criterion to safely optimize hazardous chemical processes involving arbitrary kinetic schemes. Ind Eng Chem Res 2011; 50(3):1588-89.

[21] Quin C, Chen C, Xiao Q, Yang N, Yaun C, Kulkenmann C, Cetinkaya M, Mulheim K. CFD-PBM Simulation of droplet size distribution in rotar stator mixing devices, Chem Eng Sci 2016;155:16-26.

[22] Khan MA, Ngo HH, Guo WS, Liu Y, Neghium LD, Deng LJ., Wang J, Wu Y, Optimization of process parameters in CSTR for production of volatile fatty acid, bio hydrogen and methane from anaerobic digestion. Bioresour Technol 2016; 219:738-48.

[23] Glavinc P, Kravanja Z, Homesak M. Heat integration of reactors and Criteria for the placement of reactors into process flow sheet. Chem Eng Sci 1988;43(3):593-608.

[24] Glavinc P, Kravanja Z, Homesak M. Modeling of reactors for process heat integration. Comput Chem Eng 1988; 12(2):189-94.

[25] Goguca Z, Hanika J. Dynamic modelling of glucose oxidation with palladium catalyst deactivation in multifunctional CSTR; Benefits of periodic operation, cost and time consumption. Chem Eng J 2009; 150:223-30.

[26] Mireresu A, Prusse U. A new environmental friendly method for the preparation of sugar acids via catalytic oxidation on gold catalyst. Appl Catal B 2007;70:644-52.

[27] Triveni B, Vishwanadham B, Madhavi T, Venkateshwar S. Mixing studies of non-Newtonian fluids in an anchor agitated vessel. Chem Eng Res. Des 2010; 88(7):809-18.

[28] Patel D, Ein-Mozaffari F, Mehrvar M. Improving the dynamic performance of continuous-flow mixing of pseudoplastic fluids possessing yield stress using Maxblend impeller. Chem Eng Res Des 2012;90(4):514-23.

[29] Levenspiel O., Chemical Reaction Engineering, 2nd Edition, John wiley and Sons, Inc, New York; 1972.

[30] Reinecke S.F, Deutchmann A, Jobst K, Hampel U. Macro-mixing characterization

of a stirred model fermentor of non-Newtonian liquid by flow following sensor particle. Chem Eng Res Des 2016;118:1-11.

[31] Wu B, Chen S, CFD Simulation of non-Newtonian fluid flow in anaerobic digesters. Biotechnol Bioeng 2008;99:700-11.

[32] Hameed M, Nadeem S, Unsteady MHD flow of a non Newtonian fluid on a porous plate. J Math Anal Appl 2007;325:724-733.

[33] Feteceaue C, Angew Z. On some axial Couette flows of non-Newtonian fluids, Math Phys 2005;56:1098-106.

[34] Patel D, Ein-Mozaffari F, Mehrvar M. Improving the dynamic performance of continuous-flow mixing of pseudoplastic fluids possessing yield stress using Maxblend impeller. Chem Eng Res Des 2012;90(4):514-23.

[35] Fienberg M. Optimal reactor design from a geometric viewpoint – III, Critical CSTRs. Chem Eng Sci 2000;55(17):3553-65.

[36] Hugo P, Steinbach J, Stoesele F. Calculation of the Maximum Temperature in Stirred Tank Reactors in Case of a Breakdown of Cooling. Chem Eng Sci 1988;43:2147-52.

[37] Guao Z C, Hao L, Bai W S, Wang R, Investigation into Maximum Temperature of Synthesis Reaction and Accumulation in Isothermal Semi batch Processes. Ind Eng Chem Res 2015;54:5285-86.

[38] Sen S, Patil S, Argyropoulus D S. Thermal properties of PEG in copolymers, blends, 492 and composites: A Review. Green Chem 2015;17:4862-87.

[39] Nguyen TDH, Maschietti M, Åmand LH, Vamling L, Olausson S, Anderson SI. The effect of temperature on the catalytic conversion of Kraft lignin using near-critical water, Bioresourc Technol 2014; 170:196-203.

[40] He S, Ding L, Xu K, Geng J, Ren H. Effect of high temperature on highly unsaturated fatty acids biosynthesis in activated sludge using CSTR. Bioresour Technol 2016;211:494-501.

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